Intricacies of Counterflow Flames in Validating Chemical Kinetic Models

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Motivation

- Experimental data presented at the last MACCCR Meeting by Jackie Sung

![Graph showing n-Dodecane/Air, φ=1.4, $T_u \sim 400$ K]
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![Graph showing reference flame speed versus stretch rate for S-8/Air Mixtures, $T_u=400$ K.](image-url)
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Questions?

- How accurate is the local strain rate, reference velocity, ...?
- Can we use an alternate counterflow flame property for optimization and validation of chemical kinetic models?
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- Can we use an alternate counterflow flame property for optimization and validation of chemical kinetic models?

Extinction Strain Rate of Nonpremixed Flames
Outline

- A brief review

- Uncertainties of experimental data:
  - premixed flames (last MACCCR Fuels Meeting at NIST)
  - non-premixed flames (eg. ethylene-air data of USC, NASA Langley, and UVa)

- Two-dimensional effects?
  - LDV and PIV data
  - UNICORN simulations by Katta

- Mechanism reduction based on principal component/QSSA analyses

- Concluding remarks
Review - Free-floating Limit

- Ideal, free-floating counterflow field for $L/D > 2$

![Diagram of free-floating flow field]

**Ideal case**

Potter, Heimel, and Buttler
Eighth Combustion Symposium, 1960

$a_{global} \sim 1900 s^{-1}$ at $L/D \sim 1$
Review - Free-floating Limit

- Non-ideal counterflow field for $L/D < 1$

Non-ideal case

Potter, Heimel, and Buttler
Eighth Combustion Symposium, 1960

$$a_{global} \sim 1900\, s^{-1} \text{ at } L/D \sim 1$$
Review - Influence of Nozzle Exit Profile

- Non-ideal separation distance effect on nozzle exit velocity profile
- First demonstrated by Rolon et al. in early 1990’s.
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- Non-ideal separation distance effect on nozzle exit velocity profile
- First demonstrated by Rolon et al. in early 1990’s.
Review - Influence of Radial Boundary Condition

- Finite $\frac{\partial v_r}{\partial r} (\equiv U)$ (Chelliah et al., 23rd Symp., 1990, Smooke et al. 1990)
- Axial velocity of methane-air non-premixed flames near extinction
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Uncertainties – Burning Velocity of Premixed Flames

- Three key uncertainties
  - (i) local strain rate,
  - (ii) reference velocity
  - (ii) linear vs. non-linear extrapolation (Stahl, Warnatz, and Rogg, 1988).

![Graph of n-Dodecane/Air, φ=1.4, $T_u \sim 400$ K](image)

- USC
- CWRU
Some Definitions of Nonpremixed Flame Characteristics

- Global Strain Rate $a_{global} = 4 \frac{v_{air}}{L}$ (Seshadri and Williams, 1978)

where $v_{air}$ from (i) Volume/Area, (ii) LDV/PIV, and (iii) computations.
Extinction limit of ethylene-air Nonpremixed Flames

- ONE key uncertainty ⇒ measurement of strain rate!

- Experiments from USC, NASA Langley, and UVa.

- Chemical kinetic models of Wang and co-workers.

- Full Stefan-Maxwell Eq. to reduce uncertainty of diffusion
Influence of $U = 0$ vs. $U = \text{Finite}$ on Local Strain Rate

- $\frac{dv_z}{dz} + 2\rho U(z) = 0$ (Kee et al. 1988, Smooke et al., 1990)
Summary of Experimental Data and Uncertainties

- Particle seeding in LDV/PIV $\Rightarrow$ lower local strain rate?

![Graph showing strain rate vs. separation distance with data points for different conditions.]
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2D Axisymmetric Computations

- Amantini et al. (2007) considered a methane-air case
- Vish Katta’s UNICORN code with USC Mech II Optimized for ethylene-air
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Principal Component Analysis with Sensitivity (PCAS)

• Starting point of PCAS is the construction of response function (Vajda, Valko, and Turanyi (1985)):

\[
Q(P) = \sum_{j=1}^{q} \sum_{i=1}^{m} \left[ \frac{f_i(x_j, P) - f_i(x_j, P^0)}{f_i(x_j, P^0)} \right]^2
\]

where \( P, P^0 \) are unperturbed and perturbed parameters \( (k = 1, ..., p) \); \( f_i \) a set of target functions \( (i = 1, ..., m) \); \( x_j \) collection of analysis points \( (j = 1, ..., q) \).

• Around \( P^0 \), the response function can be approximated as:

\[
Q(P) \approx q(P) = (\Delta P)^T S^T S(\Delta P) = (\Delta P)^T U^T \Lambda U(\Delta P) = \sum_{k=1}^{p} \lambda_k (\Delta \Psi_k)^2
\]

where \( \Delta P = P - P^0 \); \( S \) collection of sensitivity matrices; \( \lambda_k \) eigenvalues; \( U \) normalized eigenvectors; \( \Delta \Psi = U^T P \) principal components.
Application of PCAS to Ignition Delay

- Several key issues!!!
- Ethylene-air, $p=1.0\text{atm}$, $\phi=1.0$ with Wang 2003 detailed model (71 species in 467 reactions)
Application of PCAS to Ignition Delay

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- Ethylene-air, $p=1.0\text{atm}$, $\phi=1.0$ with Wang 2003 detailed model (71 species in 467 reactions)
Application of PCAS to Flame Propagation

- Ethylene-air, $p=1.0\,\text{atm}$, $T_0=300\,\text{K}$ with Wang 2003 detailed model (71 species in 467 reactions)
Application of PCAS to Flame Extinction

- Ethylene-air, $p=1.0$ atm, $T_0=300$ K
QSSA Reduction Approach


• In the process of updating based on USC Mech II Optimized.
NIST Chemical Kinetics Database Program

- Extremely useful tool to analyze differences between chemical kinetic models (Don Burgess)

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Concluding Remarks

- In quasi 1D extinction limit computations, $U = 0$ and $U = \text{finite}$ (from actual experiments) differ by nearly 10%!!!
- In extinction experiments with convergent nozzles, $L/D = 1$ case shows a non top-hat velocity profile $\Rightarrow$ main contributor to the differences between the measured local strain rate and the global strain rate
- Random errors ($1160 \pm 20$) are too large to extract any systematic uncertainty associated with $L/D$ variation
- Detailed reaction models continue to evolve and may converge through collaborative based efforts like PrIME, this Fuels Group, ...

$\Rightarrow$ need to create accurate and independent experimental data with well-defined uncertainties

- Automated reduction procedures are needed to take advantage of the evolving detailed reaction models (PCAS/QSSA, ...)
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